Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 08:19 PM EST

PDB ID	:	1F8V
Title	:	THE STRUCTURE OF PARIACOTO VIRUS REVEALS A DODECAHEDRAL CAGE OF DUPLEX RNA
Authors	:	Tang, L.; Johnson, K.N.; Ball, L.A.; Lin, T.; Yeager, M.; Johnson, J.E.
Deposited on	:	2000-07-05
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

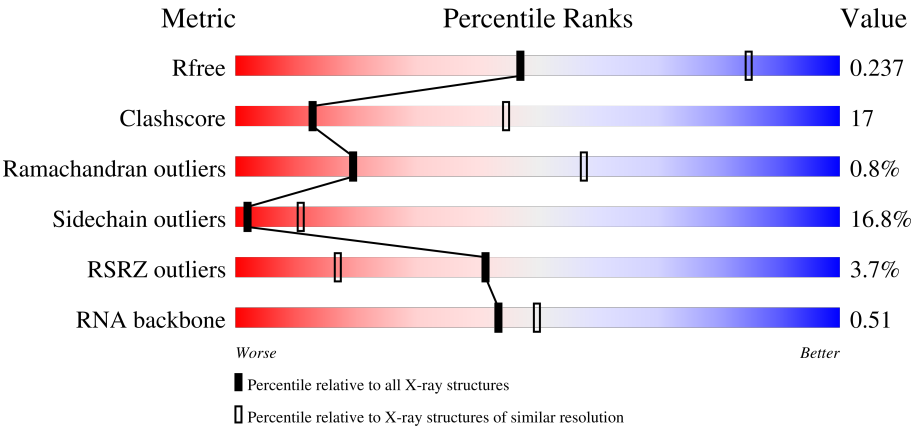
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	25	60% 40% 52% 8%
2	A	355	4% 65% 25% 10%
2	B	355	% 59% 21% 8% 12%
2	C	355	59% 21% 7% 12%

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Mol	Chain	Length	Quality of chain
3	D	40	8% 42% 12% 10% 35%
3	E	40	5% 22% 18% 15% 45%
3	F	40	5% 38% 12% 5% 45%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	C	500	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8719 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	25	509	229	62	193	25	0	0	0

- Molecule 2 is a protein called MATURE CAPSID PROTEIN BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	355	2708	1721	474	501	12	0	0	0
			Total	C	N	O	S			
2	B	313	2378	1522	396	449	11	0	0	0
			Total	C	N	O	S			
2	C	311	2363	1513	393	446	11	0	0	0

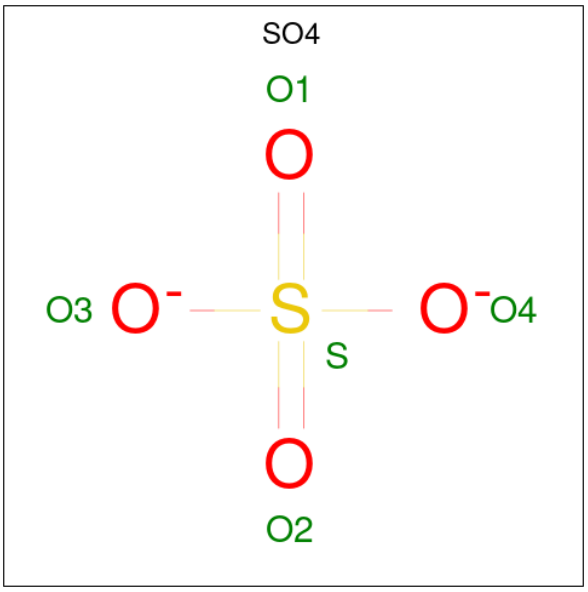
- Molecule 3 is a protein called MATURE CAPSID PROTEIN GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	26	204	130	36	36	2	0	0	1
			Total	C	N	O				
3	E	22	166	108	29	29		0	0	1
			Total	C	N	O				
3	F	22	166	108	29	29		0	0	1

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

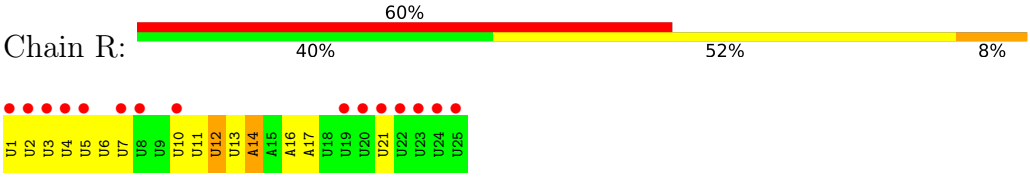
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	R	2	Total O 2 2	0	0
6	A	77	Total O 77 77	0	0
6	D	2	Total O 2 2	0	0
6	B	60	Total O 60 60	0	0
6	C	76	Total O 76 76	0	0
6	F	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

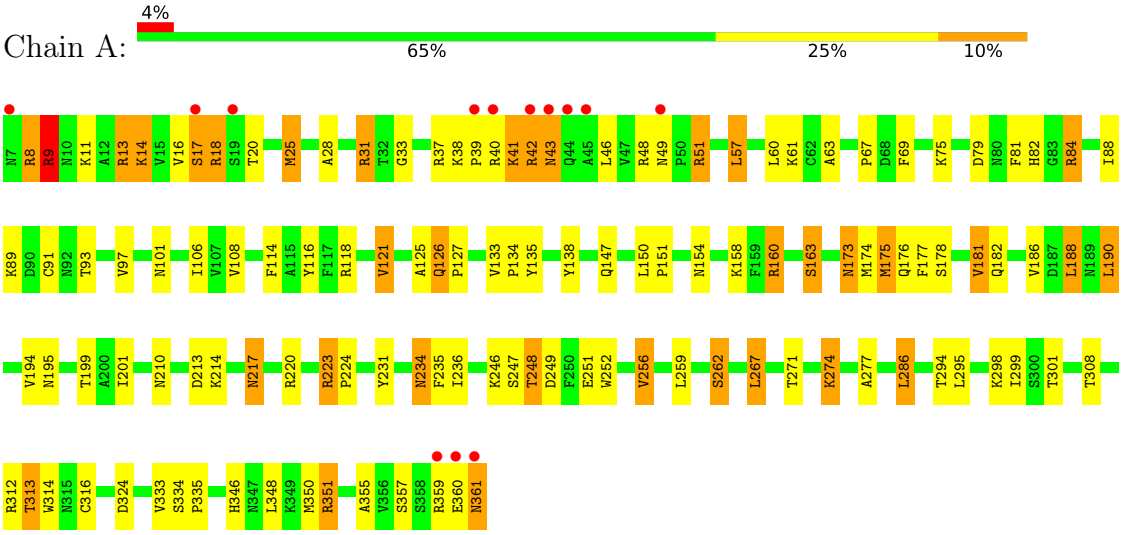
• Molecule 1: RNA

Chain R:



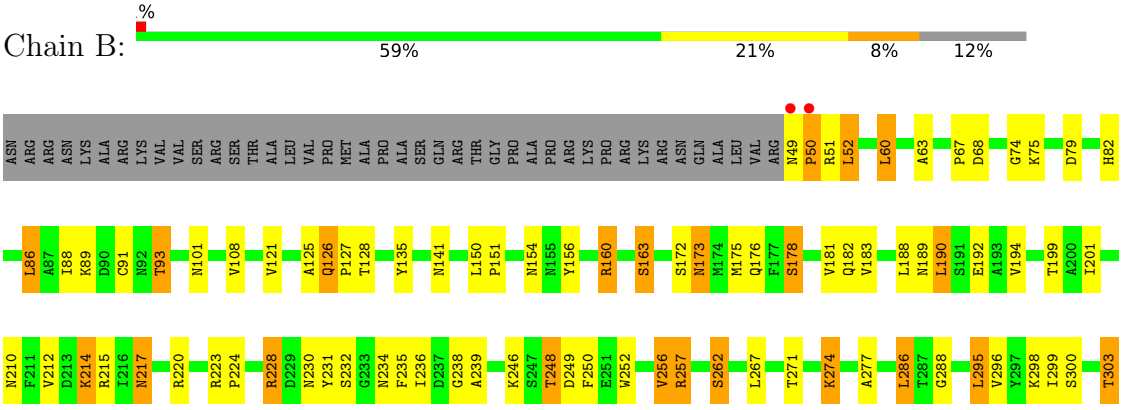
• Molecule 2: MATURE CAPSID PROTEIN BETA

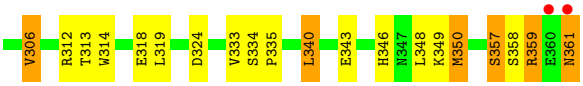
Chain A:



• Molecule 2: MATURE CAPSID PROTEIN BETA

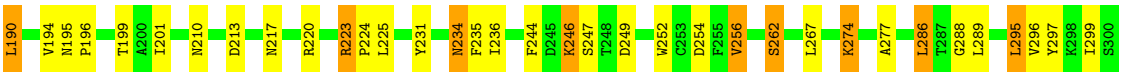
Chain B:

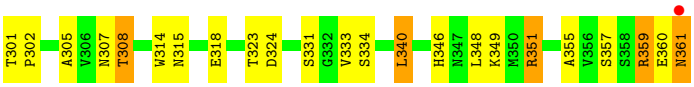




• Molecule 2: MATURE CAPSID PROTEIN BETA

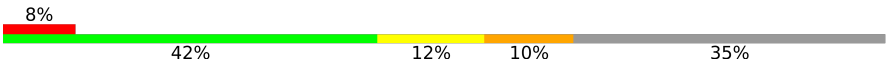
Chain C:

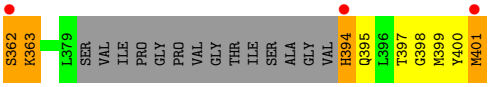




• Molecule 3: MATURE CAPSID PROTEIN GAMMA

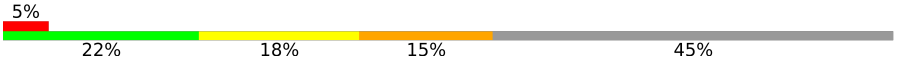
Chain D:

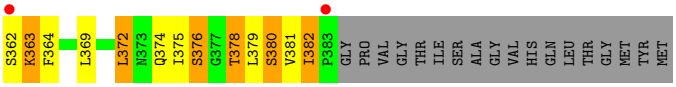




• Molecule 3: MATURE CAPSID PROTEIN GAMMA

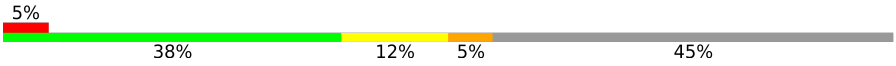
Chain E:

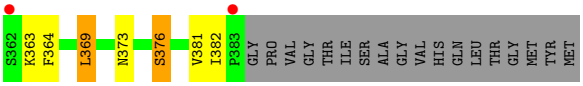




• Molecule 3: MATURE CAPSID PROTEIN GAMMA

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	329.33Å 346.94Å 424.89Å 90.00° 90.83° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 207.27 – 3.02	Depositor EDS
% Data completeness (in resolution range)	65.6 (20.00-3.00) 80.7 (207.27-3.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.21 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.219 , 0.221 0.237 , 0.237	Depositor DCC
R_{free} test set	150647 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8719	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	R	0.46	1/562 (0.2%)	0.69	0/866
2	A	0.44	0/2779	0.68	1/3792 (0.0%)
2	B	0.45	0/2444	0.69	1/3342 (0.0%)
2	C	0.44	0/2428	0.69	1/3319 (0.0%)
3	D	0.54	0/207	0.55	0/275
3	E	0.55	0/168	0.59	0/227
3	F	0.55	0/168	0.60	0/227
All	All	0.45	1/8756 (0.0%)	0.68	3/12048 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1	U	OP3-P	-7.16	1.52	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	247	SER	N-CA-C	-5.41	96.39	111.00
2	B	86	LEU	N-CA-C	-5.21	96.92	111.00
2	C	247	SER	N-CA-C	-5.07	97.32	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	509	0	255	13	0
2	A	2708	0	2672	111	0
2	B	2378	0	2305	86	0
2	C	2363	0	2292	72	0
3	D	204	0	200	9	0
3	E	166	0	174	18	0
3	F	166	0	174	6	0
4	A	1	0	0	0	0
5	C	5	0	0	0	0
6	A	77	0	0	2	0
6	B	60	0	0	4	0
6	C	76	0	0	3	0
6	D	2	0	0	0	0
6	F	2	0	0	0	0
6	R	2	0	0	0	0
All	All	8719	0	8072	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:11:U:H3'	1:R:12:U:H5"	1.30	1.11
2:B:173:ASN:HD22	2:B:175:MET:H	1.06	1.03
2:A:121:VAL:HG13	2:A:125:ALA:HB3	1.48	0.96
2:A:173:ASN:H	2:A:176:GLN:HE21	1.12	0.95
2:C:262:SER:HB2	2:C:274:LYS:HB3	1.51	0.93
2:B:176:GLN:HB2	2:B:306:VAL:HG13	1.50	0.93
2:B:262:SER:HB2	2:B:274:LYS:HB3	1.49	0.93
2:B:93:THR:HG23	2:B:312:ARG:HG2	1.49	0.93
2:A:8:ARG:HA	2:A:8:ARG:HH11	1.34	0.92
2:B:121:VAL:HG13	2:B:125:ALA:HB3	1.50	0.92
2:A:173:ASN:HD22	2:A:175:MET:H	1.16	0.91
2:A:361:ASN:HB3	3:D:363:LYS:HD3	1.52	0.89
2:B:173:ASN:ND2	2:B:175:MET:H	1.71	0.88
2:C:173:ASN:HD22	2:C:175:MET:H	1.21	0.88
2:C:121:VAL:HG13	2:C:125:ALA:HB3	1.58	0.85
2:B:49:ASN:HB3	2:B:50:PRO:HD3	1.59	0.85
2:A:49:ASN:HB3	3:F:382:ILE:HD11	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ASP:HB3	3:E:363:LYS:HE2	1.62	0.81
2:C:181:VAL:HG22	2:C:235:PHE:HA	1.64	0.79
2:A:173:ASN:ND2	2:A:175:MET:H	1.81	0.79
2:B:234:ASN:HD22	2:B:236:ILE:H	1.32	0.78
2:A:93:THR:HG23	2:A:312:ARG:HG2	1.67	0.77
2:A:51:ARG:O	2:A:51:ARG:HD3	1.84	0.77
2:C:223:ARG:HD2	6:C:524:HOH:O	1.84	0.77
2:C:361:ASN:H	2:C:361:ASN:ND2	1.83	0.75
2:A:46:LEU:HG	3:F:381:VAL:HG11	1.66	0.75
2:B:223:ARG:HB2	2:B:224:PRO:HD2	1.71	0.73
2:B:248:THR:HB	2:B:249:ASP:OD2	1.89	0.73
2:A:262:SER:HB2	2:A:274:LYS:CB	2.18	0.73
1:R:11:U:H3'	1:R:12:U:C5'	2.15	0.72
1:R:11:U:C3'	1:R:12:U:H5"	2.16	0.72
2:B:182:GLN:OE1	2:B:298:LYS:HE2	1.89	0.72
2:A:181:VAL:CG2	2:A:235:PHE:HA	2.20	0.72
2:A:173:ASN:N	2:A:176:GLN:HE21	1.86	0.71
2:B:361:ASN:O	3:E:364:PHE:HB2	1.89	0.71
2:A:14:LYS:HE3	2:A:28:ALA:HB2	1.72	0.70
2:C:63:ALA:HA	2:C:163:SER:HB2	1.71	0.70
2:A:262:SER:HB2	2:A:274:LYS:HB2	1.73	0.70
2:C:361:ASN:H	2:C:361:ASN:HD22	1.37	0.70
3:D:399:MET:HG2	3:E:379:LEU:HB3	1.74	0.69
2:C:262:SER:HB2	2:C:274:LYS:CB	2.22	0.69
2:A:223:ARG:HD2	6:A:527:HOH:O	1.93	0.68
2:C:181:VAL:CG2	2:C:235:PHE:HA	2.23	0.68
2:B:63:ALA:HA	2:B:163:SER:HB2	1.76	0.67
2:A:182:GLN:OE1	2:A:298:LYS:HE2	1.95	0.67
2:A:181:VAL:HG22	2:A:235:PHE:HA	1.77	0.67
2:B:52:LEU:HD13	2:B:340:LEU:HD13	1.77	0.66
2:C:223:ARG:HB2	2:C:224:PRO:HD2	1.78	0.66
2:A:210:ASN:HD21	2:B:267:LEU:HD13	1.60	0.65
2:A:42:ARG:HG3	3:E:376:SER:HB2	1.78	0.65
1:R:6:U:H2'	1:R:7:U:O4'	1.96	0.64
1:R:4:U:H5'	2:A:13:ARG:NH1	2.13	0.64
2:A:248:THR:HG21	2:B:160:ARG:NH2	2.11	0.64
2:A:220:ARG:HD2	2:B:324:ASP:OD2	1.98	0.63
2:A:31:ARG:O	2:B:228:ARG:HD2	1.99	0.63
2:C:361:ASN:OXT	3:F:364:PHE:HB2	1.99	0.63
2:A:31:ARG:HD3	2:A:33:GLY:O	1.99	0.63
1:R:4:U:H5'	2:A:13:ARG:HH12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:57:LEU:HD13	2:A:61:LYS:HE2	1.80	0.62
1:R:13:U:H2'	1:R:14:A:O4'	1.99	0.62
2:A:154:ASN:O	2:C:220:ARG:NH2	2.32	0.62
2:A:324:ASP:OD2	2:C:220:ARG:HD2	1.99	0.62
2:B:262:SER:HB2	2:B:274:LYS:CB	2.26	0.62
2:C:84:ARG:HG2	2:C:84:ARG:HH11	1.65	0.62
2:A:8:ARG:NH1	2:A:9:ARG:H	1.99	0.61
2:B:49:ASN:HB2	3:E:380:SER:HB3	1.81	0.61
2:A:79:ASP:OD2	2:A:160:ARG:NH2	2.33	0.61
2:B:173:ASN:HD22	2:B:173:ASN:C	2.04	0.61
2:C:79:ASP:OD2	2:C:160:ARG:NH2	2.33	0.61
1:R:11:U:H2'	1:R:12:U:O4'	2.02	0.60
2:A:93:THR:HG23	2:A:312:ARG:CG	2.32	0.60
2:A:217:ASN:N	2:A:217:ASN:HD22	1.99	0.60
2:A:223:ARG:HB2	2:A:224:PRO:HD2	1.84	0.60
2:B:121:VAL:CG1	2:B:125:ALA:HB3	2.29	0.60
2:C:84:ARG:HH11	2:C:84:ARG:CG	2.15	0.60
2:B:359:ARG:HB2	2:B:359:ARG:CZ	2.32	0.60
3:D:397:THR:O	3:D:399:MET:N	2.35	0.59
2:A:234:ASN:HD22	2:A:236:ILE:H	1.51	0.59
2:B:334:SER:HB2	2:B:335:PRO:HD2	1.85	0.59
2:A:63:ALA:HA	2:A:163:SER:HB2	1.83	0.59
2:C:277:ALA:HB2	2:C:286:LEU:HD13	1.85	0.59
2:B:217:ASN:N	2:B:217:ASN:HD22	2.00	0.59
2:C:173:ASN:ND2	2:C:175:MET:H	1.95	0.59
2:B:181:VAL:CG2	2:B:235:PHE:HA	2.33	0.58
2:B:239:ALA:N	2:B:358:SER:HB3	2.19	0.58
2:B:93:THR:HG23	2:B:312:ARG:CG	2.29	0.58
2:B:201:ILE:HG12	6:B:363:HOH:O	2.03	0.58
2:A:84:ARG:HG2	2:A:84:ARG:HH11	1.69	0.58
3:F:373:ASN:O	3:F:376:SER:HB2	2.04	0.58
2:A:173:ASN:ND2	2:A:176:GLN:H	2.02	0.57
2:A:201:ILE:HG12	6:B:362:HOH:O	2.04	0.57
2:A:39:PRO:HG2	3:E:374:GLN:HE21	1.69	0.57
2:A:262:SER:HB2	2:A:274:LYS:HB3	1.84	0.57
2:C:52:LEU:CD1	2:C:340:LEU:HD13	2.35	0.56
2:A:210:ASN:ND2	2:B:267:LEU:HD13	2.19	0.56
3:D:362:SER:N	3:D:363:LYS:HE3	2.20	0.56
3:D:363:LYS:H	3:D:363:LYS:CD	2.16	0.56
2:C:158:LYS:HD2	2:C:254:ASP:OD2	2.06	0.56
2:A:173:ASN:H	2:A:176:GLN:NE2	1.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:324:ASP:HB2	2:C:223:ARG:HE	1.70	0.56
2:C:361:ASN:C	3:F:364:PHE:HB2	2.26	0.56
2:A:121:VAL:CG1	2:A:125:ALA:HB3	2.31	0.56
2:B:220:ARG:NH2	2:C:154:ASN:O	2.39	0.56
2:A:177:PHE:CD1	2:A:178:SER:N	2.75	0.55
2:A:126:GLN:OE1	2:A:223:ARG:HB3	2.07	0.55
2:A:42:ARG:HG3	3:E:376:SER:CB	2.35	0.55
2:B:181:VAL:HG23	2:B:235:PHE:HA	1.89	0.55
2:B:194:VAL:HG12	2:B:210:ASN:HB3	1.89	0.55
2:A:67:PRO:HB3	2:A:314:TRP:CZ2	2.42	0.54
2:A:262:SER:CB	2:A:274:LYS:HB2	2.37	0.54
2:C:217:ASN:N	2:C:217:ASN:HD22	2.05	0.54
2:A:220:ARG:NH2	2:B:154:ASN:O	2.40	0.54
2:A:194:VAL:HG12	2:A:210:ASN:HB3	1.91	0.53
2:B:220:ARG:HD2	2:C:324:ASP:OD2	2.09	0.53
2:B:67:PRO:HB3	2:B:314:TRP:CZ2	2.43	0.53
2:B:249:ASP:OD2	2:B:249:ASP:N	2.42	0.53
1:R:16:A:O2'	1:R:17:A:H5'	2.09	0.53
2:B:306:VAL:O	2:B:306:VAL:HG22	2.09	0.53
2:C:61:LYS:HD3	2:C:69:PHE:CZ	2.44	0.53
2:C:84:ARG:HG2	2:C:84:ARG:NH1	2.19	0.53
2:C:195:ASN:ND2	2:C:213:ASP:OD1	2.39	0.52
6:A:502:HOH:O	2:C:201:ILE:HG12	2.09	0.52
2:A:49:ASN:HD22	2:A:51:ARG:HG3	1.75	0.52
2:C:256:VAL:HG22	2:C:256:VAL:O	2.09	0.52
2:C:299:ILE:HD12	2:C:299:ILE:N	2.24	0.52
2:A:299:ILE:HD12	2:A:299:ILE:N	2.25	0.52
2:A:231:TYR:CB	2:A:355:ALA:HB3	2.40	0.52
2:B:74:GLY:O	2:B:89:LYS:HD3	2.09	0.52
2:A:259:LEU:HD23	2:A:267:LEU:HD11	1.92	0.51
2:B:346:HIS:HA	2:B:349:LYS:HE2	1.91	0.51
2:A:8:ARG:NH1	2:A:9:ARG:N	2.59	0.51
2:A:195:ASN:ND2	2:A:213:ASP:OD2	2.42	0.51
2:A:361:ASN:N	2:A:361:ASN:HD22	2.10	0.50
2:B:249:ASP:O	2:B:250:PHE:HB2	2.10	0.50
2:C:249:ASP:OD1	2:C:249:ASP:N	2.45	0.50
2:A:48:ARG:NH1	3:D:400:TYR:O	2.39	0.50
2:A:135:TYR:OH	2:A:313:THR:HG22	2.12	0.49
2:B:79:ASP:OD2	2:B:160:ARG:NH2	2.40	0.49
2:B:160:ARG:HD2	2:B:252:TRP:CE2	2.47	0.49
2:A:249:ASP:OD2	2:A:249:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:LEU:HA	2:C:351:ARG:HG3	1.95	0.49
2:A:234:ASN:ND2	2:A:236:ILE:HG22	2.28	0.48
2:C:357:SER:OG	2:C:359:ARG:HG3	2.12	0.48
2:A:49:ASN:HD22	2:A:51:ARG:CG	2.27	0.48
2:B:277:ALA:HB2	2:B:286:LEU:HD13	1.95	0.48
2:C:231:TYR:CB	2:C:355:ALA:HB3	2.44	0.48
2:A:361:ASN:CB	3:D:363:LYS:HD3	2.36	0.48
2:B:350:MET:HG2	2:C:333:VAL:HG13	1.95	0.48
2:C:97:VAL:HG22	2:C:308:THR:CG2	2.43	0.48
1:R:11:U:H2'	1:R:12:U:C4'	2.44	0.48
2:C:177:PHE:CZ	2:C:236:ILE:HB	2.49	0.48
2:C:160:ARG:NH1	2:C:318:GLU:OE1	2.44	0.48
2:C:177:PHE:CD1	2:C:178:SER:N	2.82	0.48
2:A:277:ALA:HB2	2:A:286:LEU:HD13	1.95	0.48
2:A:88:ILE:O	2:A:316:CYS:HA	2.14	0.47
2:A:91:CYS:HB2	2:A:314:TRP:CD1	2.49	0.47
2:A:173:ASN:CG	2:A:176:GLN:HG2	2.35	0.47
1:R:5:U:O2'	1:R:6:U:H5'	2.15	0.47
2:C:301:THR:HG23	2:C:307:ASN:ND2	2.29	0.47
2:A:194:VAL:CG1	2:A:210:ASN:HB3	2.44	0.47
3:D:394:HIS:HB3	3:D:395:GLN:H	1.47	0.47
2:B:126:GLN:NE2	2:B:127:PRO:O	2.48	0.47
1:R:2:U:O2'	1:R:3:U:H5'	2.14	0.47
1:R:11:U:C3'	1:R:12:U:C5'	2.86	0.47
2:A:81:PHE:HE1	2:C:246:LYS:O	1.98	0.47
2:B:49:ASN:HB3	2:B:50:PRO:CD	2.37	0.47
2:C:72:ASP:OD1	2:C:89:LYS:HE2	2.15	0.47
2:A:61:LYS:HB3	2:A:69:PHE:CE1	2.50	0.47
2:A:91:CYS:HA	2:A:313:THR:O	2.14	0.47
2:A:173:ASN:HD21	2:A:176:GLN:H	1.60	0.47
2:A:42:ARG:CZ	3:E:376:SER:HA	2.45	0.47
2:B:173:ASN:ND2	2:B:173:ASN:C	2.67	0.47
2:C:183:VAL:HA	2:C:296:VAL:O	2.15	0.47
2:A:160:ARG:HD2	2:A:252:TRP:CE2	2.50	0.46
3:E:381:VAL:HG12	3:E:382:ILE:H	1.79	0.46
2:A:346:HIS:O	2:B:82:HIS:HD2	1.97	0.46
2:B:86:LEU:HD12	2:B:86:LEU:HA	1.82	0.46
2:B:359:ARG:HB2	2:B:359:ARG:NH1	2.31	0.46
2:C:302:PRO:HG2	2:C:305:ALA:HB2	1.98	0.46
2:B:160:ARG:HD3	2:B:318:GLU:OE1	2.15	0.46
2:C:126:GLN:NE2	2:C:127:PRO:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:150:LEU:HB3	2:A:151:PRO:HD2	1.97	0.46
3:E:372:LEU:HD22	3:E:372:LEU:O	2.15	0.46
2:C:288:GLY:HA3	6:C:529:HOH:O	2.15	0.46
2:B:141:ASN:ND2	2:B:156:TYR:OH	2.49	0.45
3:F:369:LEU:HD12	3:F:369:LEU:HA	1.82	0.45
2:B:299:ILE:N	2:B:299:ILE:HD12	2.31	0.45
2:B:343:GLU:OE2	3:E:378:THR:HB	2.17	0.45
2:B:234:ASN:ND2	2:B:236:ILE:H	2.07	0.45
2:C:173:ASN:ND2	2:C:176:GLN:H	2.15	0.45
2:A:116:TYR:CZ	2:A:133:VAL:HG21	2.51	0.45
2:A:8:ARG:HA	2:A:8:ARG:NH1	2.17	0.45
2:A:256:VAL:HG22	2:A:256:VAL:O	2.16	0.45
2:A:8:ARG:HA	2:A:8:ARG:HD2	1.48	0.45
2:A:108:VAL:O	2:A:294:THR:HG23	2.17	0.45
2:C:84:ARG:HA	2:C:84:ARG:HD3	1.77	0.45
2:C:108:VAL:HB	2:C:295:LEU:HB2	1.98	0.45
2:C:234:ASN:ND2	2:C:236:ILE:HG22	2.32	0.45
2:B:88:ILE:HD12	2:B:319:LEU:HD11	1.99	0.45
2:A:234:ASN:ND2	2:A:236:ILE:H	2.13	0.44
3:D:401:MET:HE3	6:B:420:HOH:O	2.18	0.44
2:C:194:VAL:CG1	2:C:210:ASN:HB3	2.47	0.44
2:A:17:SER:O	2:A:18:ARG:O	2.35	0.44
2:B:160:ARG:NH1	2:B:318:GLU:OE1	2.43	0.44
2:B:348:LEU:HD11	3:E:372:LEU:HD23	1.99	0.44
2:B:101:ASN:HB2	2:B:303:THR:HG23	1.99	0.44
2:B:357:SER:OG	2:B:359:ARG:HD3	2.18	0.44
2:C:244:PHE:CD1	2:C:349:LYS:HD2	2.53	0.44
2:B:172:SER:HB3	2:B:176:GLN:HG3	2.00	0.44
2:C:82:HIS:HA	2:C:334:SER:HB3	1.99	0.44
2:C:84:ARG:HD2	2:C:331:SER:HB2	2.00	0.44
2:A:267:LEU:HD22	2:C:210:ASN:OD1	2.18	0.43
2:C:182:GLN:HA	2:C:231:TYR:O	2.19	0.43
2:A:186:VAL:HG23	2:A:188:LEU:HD13	1.99	0.43
2:C:150:LEU:HB3	2:C:151:PRO:HD2	2.00	0.43
2:C:160:ARG:HD2	2:C:252:TRP:CE2	2.53	0.43
2:B:173:ASN:ND2	2:B:175:MET:N	2.53	0.43
2:C:121:VAL:CG1	2:C:125:ALA:HB3	2.39	0.43
2:B:214:LYS:C	2:B:215:ARG:HG2	2.39	0.43
2:A:158:LYS:HD3	2:A:252:TRP:HB3	2.01	0.43
2:A:106:ILE:HD13	2:A:118:ARG:HG3	2.01	0.43
2:B:256:VAL:O	2:B:256:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:363:LYS:H	3:E:363:LYS:HG3	1.38	0.43
2:A:84:ARG:HG2	2:A:84:ARG:NH1	2.33	0.43
2:B:135:TYR:OH	2:B:313:THR:HG22	2.19	0.43
2:B:238:GLY:HA3	2:B:358:SER:HB3	2.00	0.43
2:C:52:LEU:HD13	2:C:340:LEU:HD13	1.99	0.43
2:A:82:HIS:HD2	2:C:346:HIS:O	2.02	0.43
2:B:192:GLU:HG3	2:B:214:LYS:HE3	2.01	0.42
2:C:314:TRP:O	2:C:315:ASN:HB3	2.18	0.42
2:A:182:GLN:HA	2:A:231:TYR:O	2.18	0.42
2:A:334:SER:HB2	2:A:335:PRO:CD	2.50	0.42
2:B:234:ASN:ND2	2:B:236:ILE:HG22	2.34	0.42
2:A:41:LYS:HB2	2:A:43:ASN:ND2	2.34	0.42
2:A:234:ASN:HD22	2:A:236:ILE:N	2.17	0.42
2:B:91:CYS:HB2	2:B:314:TRP:CD1	2.54	0.42
2:B:150:LEU:HB3	2:B:151:PRO:HD2	2.02	0.42
2:C:106:ILE:HB	2:C:297:TYR:HB2	2.02	0.42
3:E:369:LEU:HD23	3:E:369:LEU:HA	1.82	0.42
2:A:126:GLN:NE2	2:A:127:PRO:O	2.53	0.42
2:A:267:LEU:HD12	2:A:267:LEU:HA	1.90	0.42
2:B:91:CYS:HA	2:B:313:THR:O	2.19	0.42
2:B:234:ASN:HD22	2:B:236:ILE:N	2.09	0.42
2:A:348:LEU:HA	2:A:351:ARG:HG3	2.01	0.42
2:B:108:VAL:HB	2:B:295:LEU:HB2	2.01	0.42
2:A:42:ARG:NH2	3:E:375:ILE:O	2.53	0.42
2:A:42:ARG:HE	3:E:376:SER:HB3	1.83	0.42
2:B:60:LEU:HD12	2:B:60:LEU:HA	1.93	0.42
2:B:256:VAL:HG13	2:B:288:GLY:HA2	2.02	0.42
2:A:334:SER:HB2	2:A:335:PRO:HD2	2.02	0.41
2:A:61:LYS:HD2	2:A:69:PHE:CZ	2.54	0.41
2:C:86:LEU:HG	2:C:88:ILE:HD13	2.03	0.41
2:A:177:PHE:CZ	2:A:236:ILE:HB	2.54	0.41
2:C:223:ARG:HB2	2:C:223:ARG:HH11	1.84	0.41
2:A:25:MET:O	2:A:25:MET:HG3	2.16	0.41
2:C:65:ALA:C	2:C:67:PRO:HD2	2.40	0.41
2:C:190:LEU:HD13	2:C:289:LEU:HD22	2.03	0.41
2:A:42:ARG:NE	3:E:376:SER:HB3	2.36	0.41
2:A:138:TYR:C	2:A:138:TYR:CD2	2.94	0.41
2:C:116:TYR:CZ	2:C:133:VAL:HG21	2.56	0.41
2:A:217:ASN:N	2:A:217:ASN:ND2	2.67	0.41
2:A:101:ASN:N	2:A:301:THR:O	2.54	0.41
2:A:114:PHE:HA	2:A:134:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:190:LEU:HD12	2:A:190:LEU:HA	1.89	0.41
2:B:343:GLU:HG3	6:B:420:HOH:O	2.21	0.41
2:A:97:VAL:HG13	2:A:308:THR:HG22	2.02	0.40
2:B:183:VAL:HA	2:B:296:VAL:O	2.22	0.40
2:B:257:ARG:HA	2:B:286:LEU:O	2.21	0.40
2:C:82:HIS:HB2	6:C:512:HOH:O	2.21	0.40
2:B:189:ASN:CG	2:C:158:LYS:HD3	2.42	0.40
2:B:217:ASN:N	2:B:217:ASN:ND2	2.68	0.40
2:B:176:GLN:HB2	2:B:306:VAL:CG1	2.37	0.40
2:B:361:ASN:C	3:E:364:PHE:HB2	2.42	0.40
2:B:190:LEU:HD12	2:B:190:LEU:HA	1.87	0.40
2:B:361:ASN:HD22	2:B:361:ASN:HA	1.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	353/355 (99%)	332 (94%)	17 (5%)	4 (1%)	14 50
2	B	311/355 (88%)	292 (94%)	17 (6%)	2 (1%)	25 64
2	C	309/355 (87%)	295 (96%)	13 (4%)	1 (0%)	41 76
3	D	22/40 (55%)	20 (91%)	1 (4%)	1 (4%)	2 14
3	E	20/40 (50%)	19 (95%)	1 (5%)	0	100 100
3	F	20/40 (50%)	19 (95%)	1 (5%)	0	100 100
All	All	1035/1185 (87%)	977 (94%)	50 (5%)	8 (1%)	19 57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	16	VAL

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Mol	Chain	Res	Type
2	A	18	ARG
3	D	398	GLY
2	A	9	ARG
2	A	360	GLU
2	B	178	SER
2	B	50	PRO
2	C	360	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	290/290 (100%)	236 (81%)	54 (19%)	1 8
2	B	255/290 (88%)	216 (85%)	39 (15%)	2 13
2	C	253/290 (87%)	216 (85%)	37 (15%)	3 15
3	D	22/33 (67%)	18 (82%)	4 (18%)	1 9
3	E	19/33 (58%)	12 (63%)	7 (37%)	0 0
3	F	19/33 (58%)	16 (84%)	3 (16%)	2 12
All	All	858/969 (88%)	714 (83%)	144 (17%)	2 11

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	8	ARG
2	A	9	ARG
2	A	11	LYS
2	A	13	ARG
2	A	14	LYS
2	A	17	SER
2	A	20	THR
2	A	25	MET
2	A	31	ARG
2	A	37	ARG
2	A	38	LYS

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Mol	Chain	Res	Type
2	A	40	ARG
2	A	41	LYS
2	A	42	ARG
2	A	43	ASN
2	A	51	ARG
2	A	57	LEU
2	A	60	LEU
2	A	75	LYS
2	A	84	ARG
2	A	89	LYS
2	A	121	VAL
2	A	126	GLN
2	A	147	GLN
2	A	160	ARG
2	A	163	SER
2	A	173	ASN
2	A	174	MET
2	A	175	MET
2	A	181	VAL
2	A	188	LEU
2	A	190	LEU
2	A	199	THR
2	A	214	LYS
2	A	217	ASN
2	A	223	ARG
2	A	234	ASN
2	A	246	LYS
2	A	248	THR
2	A	251	GLU
2	A	256	VAL
2	A	262	SER
2	A	267	LEU
2	A	271	THR
2	A	274	LYS
2	A	286	LEU
2	A	295	LEU
2	A	313	THR
2	A	333	VAL
2	A	350	MET
2	A	351	ARG
2	A	357	SER
2	A	359	ARG

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Mol	Chain	Res	Type
2	A	361	ASN
3	D	362	SER
3	D	363	LYS
3	D	394	HIS
3	D	401	MET
2	B	51	ARG
2	B	52	LEU
2	B	60	LEU
2	B	75	LYS
2	B	93	THR
2	B	126	GLN
2	B	128	THR
2	B	160	ARG
2	B	163	SER
2	B	173	ASN
2	B	178	SER
2	B	188	LEU
2	B	190	LEU
2	B	199	THR
2	B	212	VAL
2	B	214	LYS
2	B	217	ASN
2	B	228	ARG
2	B	230	ASN
2	B	231	TYR
2	B	232	SER
2	B	246	LYS
2	B	248	THR
2	B	256	VAL
2	B	257	ARG
2	B	262	SER
2	B	271	THR
2	B	274	LYS
2	B	286	LEU
2	B	295	LEU
2	B	300	SER
2	B	303	THR
2	B	306	VAL
2	B	333	VAL
2	B	340	LEU
2	B	350	MET
2	B	357	SER

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Mol	Chain	Res	Type
2	B	359	ARG
2	B	361	ASN
3	E	362	SER
3	E	363	LYS
3	E	372	LEU
3	E	376	SER
3	E	378	THR
3	E	380	SER
3	E	382	ILE
2	C	52	LEU
2	C	54	ASP
2	C	60	LEU
2	C	84	ARG
2	C	88	ILE
2	C	89	LYS
2	C	101	ASN
2	C	121	VAL
2	C	126	GLN
2	C	140	THR
2	C	147	GLN
2	C	158	LYS
2	C	160	ARG
2	C	163	SER
2	C	172	SER
2	C	176	GLN
2	C	181	VAL
2	C	188	LEU
2	C	190	LEU
2	C	196	PRO
2	C	199	THR
2	C	223	ARG
2	C	225	LEU
2	C	234	ASN
2	C	246	LYS
2	C	256	VAL
2	C	262	SER
2	C	267	LEU
2	C	274	LYS
2	C	286	LEU
2	C	295	LEU
2	C	308	THR
2	C	323	THR

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Mol	Chain	Res	Type
2	C	340	LEU
2	C	351	ARG
2	C	359	ARG
2	C	361	ASN
3	F	363	LYS
3	F	369	LEU
3	F	376	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	43	ASN
2	A	82	HIS
2	A	101	ASN
2	A	141	ASN
2	A	173	ASN
2	A	176	GLN
2	A	210	ASN
2	A	217	ASN
2	A	234	ASN
2	A	329	GLN
2	A	361	ASN
3	D	373	ASN
2	B	49	ASN
2	B	82	HIS
2	B	141	ASN
2	B	173	ASN
2	B	217	ASN
2	B	234	ASN
2	B	329	GLN
2	B	361	ASN
3	E	374	GLN
2	C	82	HIS
2	C	101	ASN
2	C	126	GLN
2	C	141	ASN
2	C	173	ASN
2	C	217	ASN
2	C	234	ASN
2	C	361	ASN
3	F	373	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	24/25 (96%)	4 (16%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	10	U
1	R	12	U
1	R	14	A
1	R	21	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	C	500	-	4,4,4	0.24	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	R	25/25 (100%)	3.21	15 (60%) 0 0	89, 182, 229, 229	0
2	A	355/355 (100%)	0.06	13 (3%) 41 17	11, 19, 70, 117	0
2	B	313/355 (88%)	-0.10	4 (1%) 77 51	11, 19, 36, 90	0
2	C	311/355 (87%)	-0.12	1 (0%) 94 84	10, 19, 32, 82	0
3	D	26/40 (65%)	0.84	3 (11%) 4 1	27, 61, 89, 96	0
3	E	22/40 (55%)	1.00	2 (9%) 9 3	31, 58, 84, 86	0
3	F	22/40 (55%)	0.62	2 (9%) 9 3	18, 45, 61, 72	0
All	All	1074/1210 (88%)	0.09	40 (3%) 41 17	10, 19, 78, 229	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	25	U	7.5
1	R	1	U	6.6
1	R	21	U	6.3
1	R	2	U	6.2
1	R	24	U	5.9
1	R	23	U	4.9
1	R	3	U	4.6
2	B	361	ASN	4.4
2	C	361	ASN	4.4
3	F	383	PRO	4.3
1	R	20	U	4.0
2	A	43	ASN	3.9
3	E	362	SER	3.8
2	A	19	SER	3.8
2	A	360	GLU	3.7
2	A	361	ASN	3.6
2	A	42	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	R	7	U	3.3
2	B	49	ASN	3.3
1	R	22	U	3.3
1	R	4	U	3.2
2	A	40	ARG	2.9
2	B	360	GLU	2.9
3	F	362	SER	2.8
3	D	362	SER	2.8
2	A	17	SER	2.7
1	R	10	U	2.7
2	A	359	ARG	2.5
1	R	19	U	2.5
2	A	44	GLN	2.5
1	R	8	U	2.4
2	A	49	ASN	2.3
2	B	50	PRO	2.2
2	A	45	ALA	2.1
1	R	5	U	2.1
2	A	7	ASN	2.1
3	D	394	HIS	2.0
3	D	401	MET	2.0
2	A	39	PRO	2.0
3	E	383	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	C	500	5/5	0.50	0.83	189,189,189,189	5
4	CA	A	501	1/1	0.87	0.09	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.